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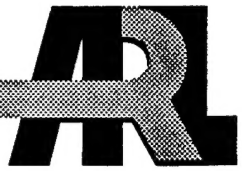
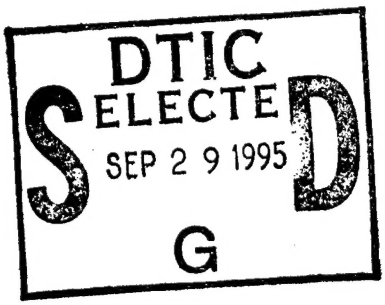


Poisson's Ratio for Poled Electroceramics

Arthur Ballato

ARL-TR-432 August 1995



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POISSON'S RATIO FOR POLED ELECTROCERAMICS

Abstract

General expressions for Poisson's ratio are derived for arbitrary orientations in hexagonal point groups; simplified forms are given for cases involving symmetry directions. Applications are made to piezoelectric ceramics.

Introduction

Poisson's ratio, ν, is defined for isotropic media as the quotient of lateral contraction to longitudinal extension arising from application of a simple tensile stress. The ratio finds application in a number of areas of applied elasticity and solid mechanics, for example, as indication of the mechanical coupling between various vibrational modes of motion. Future high-tech applications will involve mechanically resonant microstructures integrated with electronic and optical circuitry. These will require extension of Poisson's ratio considerations to a variety of crystalline and polycrystalline substances.

In most materials, the dimensionless number ν is positive. In crystals and poled electroceramics, ν takes on different values, depending on the directions of stress and strain chosen. The maximum value of $\nu = +1/2$ is obtained in the incompressible medium limit, where volume is preserved; for ordinary materials, values of +1/4 to +1/3 are typical, but in crystals ν may vanish, or take on negative values. In order to provide a synoptic yet relatively uncomplicated picture, Figure 1 sketches the bounds on ν as function of the traditional Lamé constants of an isotropic medium. Table 1 relates various elastic measures for substances or conditions indicated in the figure, or discussed in the sequel. Analytical formulas for Poisson's ratio are expressed in terms of elastic moduli. For the case of crystals of general anisotropy, these expressions are quite unwieldy, but for substances in the hexagonal system the symmetry elements reduce the complexity considerably. Many of the materials under consideration for future microdevices are characterized by hexagonal symmetry.

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The hexagonal crystal system[1-3] comprises seven point groups (6-bar m2, 622, 6mm, 6/m mm, 6-bar, 6, and 6/m), and includes a number of the binary semiconductor systems, and their alloys. These have the piezoelectric wurtzite structure; examples are GaN and AlN. The family of poled electroceramics, including $BaTiO_3$, PZT, and related alloys are characterized by symmetry ∞mm, that is, they are transversely isotropic. However, this symmetry is equivalent to 6mm for all tensor properties up to and including rank five;[4] this includes elasticity. All hexagonal groups have the same elastic matrix scheme, so for our purposes it is not necessary to distinguish between them.

Expressions Relating Hexagonal Stiffnesses and Compliances

Relations for Poisson's ratio are most simply expressed in terms of the elastic compliances $[s_{\lambda\mu}]$. It is often the case, however, that the most accurate determinations of the elastic constants (resonator and transit-time methods) yield values for the stiffnesses $[c_{\lambda\mu}]$ directly;[5] the conversion relations are given below. For the hexagonal system, the elastic stiffness and compliance matrices have identical form. Referred to the x_k axes as defined in the IEEE Standard,[5] the matrices are:

$$\begin{matrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{66} \end{matrix} \qquad \begin{matrix} s_{11} & s_{12} & s_{13} & 0 & 0 & 0 \\ s_{12} & s_{11} & s_{13} & 0 & 0 & 0 \\ s_{13} & s_{13} & s_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & s_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & s_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & s_{66} \end{matrix}$$

Stiffness and compliance are matrix reciprocals; the five independent components of each are related by:

$$(c_{11} + c_{12}) = s_{33} / S \; ; \qquad (c_{11} - c_{12}) = 1 / (s_{11} - s_{12})$$
$$c_{13} = - s_{13} / S \; ; \qquad c_{33} = (s_{11} + s_{12}) / S$$
$$c_{44} = 1 / s_{44} \; ; \qquad S = s_{33} (s_{11} + s_{12}) - 2 s_{13}^{\,2}$$

In addition, one has the relation $s_{66} = 2(s_{11} - s_{12})$. The compliances are given in terms of the stiffnesses simply by interchange of symbols, but with $c_{66} = (c_{11} - c_{12})/2$. The equality of the 11 and 22 components together with the given relations between the 66, 11 and 12 components imply transverse isotropy; that is, all directions perpendicular to the unique six-fold axis (i.e., in the basal plane) are elastically equivalent.

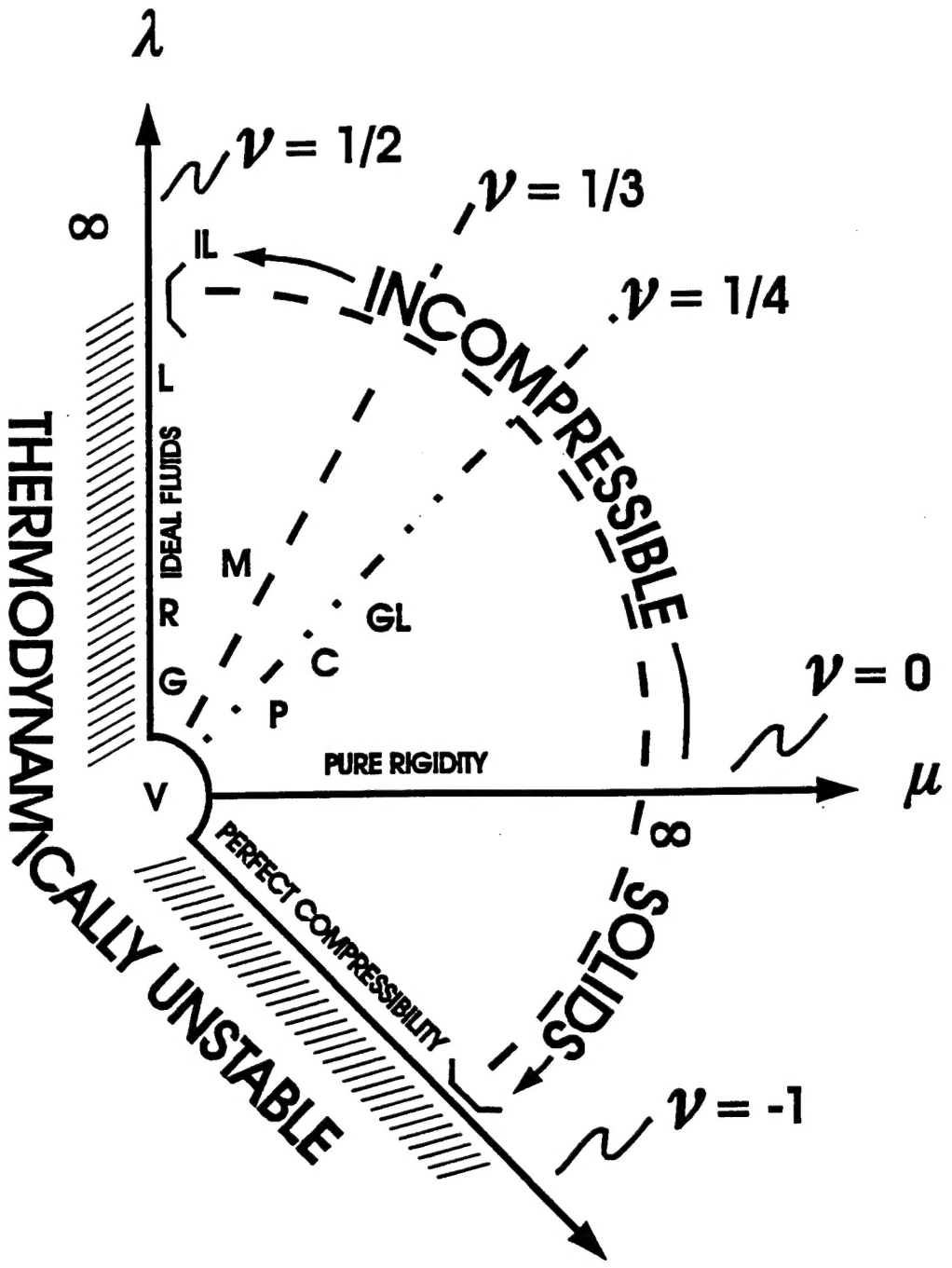

Figure 1. Limits on the Lamé constants of isotropic solids. (Symbols: C, cement; G, gas; GL, glass; IL, incompressible liquid; L, liquid; M, metal, ceramic; P, plastic; R, rubber; V, vacuum)

TABLE 1. RELATIONS AMONG ISOTROPIC ELASTIC PARAMETERS.

SUBSTANCE OR CONDITION	ν	λ	μ	Y	κ	v_{sh}/v_{long}
Ideal fluids	1/2	λ	0	0	λ	0
Many metals	1/3	2μ	μ	$8\mu/3$	$8\mu/3$	1/2
Poisson relation	1/4	μ	μ	$5\mu/2$	$5\mu/3$	$1/\sqrt{3}$
Pure rigidity	0	0	μ	2μ	$2\mu/3$	$1/\sqrt{2}$
Perfect compressibility	- 1	$-2\mu/3$	μ	0	0	$\sqrt{3}/2$
Incompressible liquids	1/2	∞	0	0	∞	0
Incompressible solids	---	∞	∞	∞	∞	---

$[v_{sh}/v_{long}]$ is ratio of shear to longitudinal wave velocities

Definition of Poisson's Ratio for Crystals

Poisson's ratio for crystals[1] is defined in general as $\nu_{ji} = - s_{ij}' / s_{jj}'$, where x_j is the direction of the longitudinal extension, x_i is the direction of the accompanying lateral contraction, and the s_{ij}' and s_{jj}' are the appropriate elastic compliances referred to this right-handed axial set. It suffices to take x_1 as the direction of the longitudinal extension; then two Poisson's ratios are defined by the orientations of the lateral axes x_2 and x_3: $\nu_{21} = - s_{12}' / s_{11}'$ and $\nu_{31} = - s_{13}' / s_{11}'$. Application of the definition requires specification of the orientation of the x_k coordinate set with respect to the crystallographic directions, and transformation of the compliances accordingly. The influence of piezoelectricity on the Poisson's ratio is neglected here, but may be incorporated in a straightforward manner. For completeness, we note that in crystals the Young's modulus Y is a function of orientation, and is defined by $s_{11}' = 1/Y$. The Lamé moduli λ, μ for isotropic elastic bodies are defined as $\lambda = c_{12} = c_{13} = c_{23}$, and $\mu = c_{44} = c_{55} = c_{66}$. The remaining nonzero isotropic stiffnesses are $(\lambda + 2\,\mu) = c_{11} = c_{22} = c_{33}$.

Relations for Rotated Hexagonal Compliances - General

The unprimed compliances are referred to a set of right-handed orthogonal axes related to the crystallographic axes in the manner defined by the IEEE standard.[5] Direction cosines a_{mn} relate the transformation from these axes to the set specifying the directions of the applied longitudinal extension (x_1), and the resulting lateral contractions (x_2 and x_3). General expressions for the transformed hexagonal compliances that enter the formulas for ν_{21} and ν_{31} are:

$$s_{11}' = s_{11}\,[a_{11}^{\,2} + a_{12}^{\,2}]^2 + s_{33}\,[a_{13}^{\,4}] + (s_{44} + 2\,s_{13})\,[a_{13}^{\,2}][a_{11}^{\,2} + a_{12}^{\,2}]$$

$$s_{12}' = s_{11}\,[a_{11}\,a_{21} + a_{12}\,a_{22}]^2 + s_{33}\,[a_{13}^{\,2}\,a_{23}^{\,2}] +$$

$$s_{44}\,[a_{13}\,a_{23}][a_{11}\,a_{21} + a_{12}\,a_{22}] + s_{12}\,[a_{11}\,a_{22} - a_{12}\,a_{21}]^2 +$$

$$s_{13}\,[a_{23}^{\,2}\,[a_{11}^{\,2} + a_{12}^{\,2}] + a_{13}^{\,2}\,[a_{21}^{\,2} + a_{22}^{\,2}]]$$

$$s_{13}' = s_{11}\,[a_{11}\,a_{31} + a_{12}\,a_{32}]^2 + s_{33}\,[a_{13}^{\,2}\,a_{33}^{\,2}] +$$

$$s_{44}\,[a_{13}\,a_{33}][a_{11}\,a_{31} + a_{12}\,a_{32}] + s_{12}\,[a_{11}\,a_{32} - a_{12}\,a_{31}]^2 +$$

$$s_{13}\,[a_{33}^{\,2}\,[a_{11}^{\,2} + a_{12}^{\,2}] + a_{13}^{\,2}\,[a_{31}^{\,2} + a_{32}^{\,2}]]$$

Transformation Matrix for General Rotations

Poisson's ratio for the most general case may be derived by considering the transformation matrix for a combination of three coordinate rotations: a first rotation about x_3 by angle φ, a second rotation about the new x_1 by angle θ, and a third rotation about the resulting x_2 by angle ψ. When these angles are set to zero, the x_1, x_2, x_3 axes coincide respectively with the reference crystallographic directions. For nonzero angles, the direction cosines a_{mn} are as follows, with the abbreviations $c(\theta)$ and $s(\theta)$ for $\cos(\theta)$ and $\sin(\theta)$, etc.:

$$\begin{matrix} [c(\varphi)c(\psi) - s(\varphi)s(\theta)s(\psi)] & [s(\varphi)c(\psi) + c(\varphi)s(\theta)s(\psi)] & [-c(\theta)s(\psi)] \\ [-s(\varphi)c(\theta)] & [c(\varphi)c(\theta)] & [\ s(\theta)\ ] \\ [c(\varphi)s(\psi) + s(\varphi)s(\theta)c(\psi)] & [s(\varphi)s(\psi) - c(\varphi)s(\theta)c(\psi)] & [\ c(\theta)c(\psi)] \end{matrix}$$

Substitution of these a_{mn} into the expressions for s_{11}' , s_{12}' , and s_{13}' , and thence into the formulas $\nu_{21} = - s_{12}' / s_{11}'$ and $\nu_{31} = - s_{13}' / s_{11}'$ formally solves the problem for specified values of φ, θ, and ψ. The condition of transverse isotropy stated above, however, renders all results independent of azimuthal angle φ, which is henceforth ignored.

Poisson's Ratios for Specific Orientations

1) Longitudinal extension in the basal plane: $\psi = 0$; θ arbitrary.
Direction cosines are: $a_{11} = 1$; $a_{22} = a_{33} = c(\theta)$; $a_{12} = - a_{21} = s(\theta)$

Rotated compliances are:

$$s_{11}' = s_{11}$$

$$s_{12}' = s_{12} \cos^2(\theta) + s_{13} \sin^2(\theta) = s_{12} + (s_{13} - s_{12}) \sin^2(\theta)$$

$$s_{13}' = s_{12} \sin^2(\theta) + s_{13} \cos^2(\theta) = s_{13} - (s_{13} - s_{12}) \sin^2(\theta)$$

Poisson's ratios are:

$$\nu_{21} = - [s_{12} + (s_{13} - s_{12}) \sin^2(\theta)] / s_{11}$$

$$\nu_{31} = - [s_{13} - (s_{13} - s_{12}) \sin^2(\theta)] / s_{11}$$

When $\theta = 0$,

$$\nu_{21} = - s_{12} / s_{11}$$

$$\nu_{31} = - s_{13} / s_{11}$$

When $\theta = \pi/4$,

$$\nu_{21} = \nu_{31} = - (s_{12} + s_{13}) / 2 s_{11}.$$

2) Longitudinal extension at an angle ψ from the basal plane; the x_2 axis in the basal plane: $\theta = 0$; ψ arbitrary.

Direction cosines are: $a_{22} = 1$; $a_{11} = a_{33} = c(\psi)$; $- a_{13} = a_{31} = s(\psi)$

Rotated compliances are:

$$s_{11}' = s_{11} [c^4(\psi)] + s_{33} [s^4(\psi)] + (s_{44} + 2 s_{13}) [c^2(\psi) s^2(\psi)]$$

$$s_{12}' = s_{12} [c^2(\psi)] + s_{13} [s^2(\psi)] = s_{12} + (s_{13} - s_{12}) [s^2(\psi)]$$

$$s_{13}' = s_{13} + s_2 [c^2(\psi) s^2(\psi)]; \; s_2 = (s_{11} + s_{33} - (s_{44} + 2 s_{13}))$$

Poisson's ratios are:

$$\nu_{21} = - s_{12}' / s_{11}'$$

$$\nu_{31} = - s_{13}' / s_{11}'.$$

When $\psi = \pi/4$,

$$\nu_{21} = - 2 (s_{12} + s_{13}) / (s_0 + s_{44})$$

$$\nu_{31} = - (s_0 - s_{44}) / (s_0 + s_{44}) \; ; \; s_0 = (s_{11} + s_{33} + 2 s_{13})$$

When $\psi = \pi/2$,

$$\nu_{21} = \nu_{31} = - s_{13} / s_{33}$$

Poisson's ratio is isotropic when the longitudinal extension is along the six-fold symmetry axis.

3) Longitudinal extension out of the basal plane: θ and ψ arbitrary.
Direction cosines are:

$[c(\psi)]$	$[\ s(\theta)s(\psi)\ ]$	$[-c(\theta)s(\psi)]$
$[\ 0\ ]$	$[\ \ c(\theta)\ \ ]$	$[\ \ s(\theta)\ \ \ ]$
$[s(\psi)]$	$[-s(\theta)c(\psi)]$	$[\ c(\theta)c(\psi)]$

Rotated compliances are:

$$s_{11}' = s_{11}\,[s^2(\theta)s^2(\psi) + c^2(\psi)]^2 + s_{33}\,[c^4(\theta)s^4(\psi)] +$$

$$(s_{44} + 2\,s_{13})\,[c^2(\theta)s^2(\psi)][s^2(\theta)s^2(\psi) + c^2(\psi)]$$

$$s_{12}' = s_{12}\,[c^2(\theta)c^2(\psi)] + s_{13}\,[s^2(\theta)c^2(\psi) + s^2(\psi)] +$$

$$s_2\,[c^2(\theta)s^2(\theta)s^2(\psi)]$$

$$s_{13}' = s_{12}\,[s^2(\theta)] + s_{13}\,[c^2(\theta)] + s_2\,[c^4(\theta)c^2(\psi)s^2(\psi)]$$

Poisson's ratios are:

$$\nu_{21} = -\,s_{12}' / s_{11}'$$

$$\nu_{31} = -\,s_{13}' / s_{11}'$$

These results reduce to those of Case 1) when $\psi = 0$, and to those of Case 2) when $\theta = 0$.

4) Longitudinal extension at an angle ψ from the basal plane: first rotation about x_2 by angle ψ, followed by a second rotation about x_1 by angle χ.
Direction cosines are:

$[\ \ c(\psi)\ ]$	$[\ \ 0\ \ ]$	$[-s(\psi)\ \ ]$
$[s(\psi)s(\chi)]$	$[\ c(\chi)]$	$[\ c(\psi)s(\chi)]$
$[s(\psi)c(\chi)]$	$[-s(\chi)]$	$[\ c(\psi)c(\chi)]$

Rotated compliances are:

$$s_{11}' = s_{11}\,[c^4(\psi)] + s_{33}\,[s^4(\psi)] + (s_{44} + 2\,s_{13})\,[c^2(\psi)s^2(\psi)]$$

$$s_{12}' = s_{12}\,[c^2(\psi)c^2(\chi)] + s_{13}\,[s^2(\psi)c^2(\chi) + s^2(\chi)] + s_2\,[c^2(\psi)s^2(\psi)s^2(\chi)]$$

$$s_{13}' = s_{12}\,[c^2(\psi)s^2(\chi)] + s_{13}\,[s^2(\psi)s^2(\chi) + c^2(\chi)] + s_2\,[c^2(\psi)s^2(\psi)c^2(\chi)]$$

Poisson's ratios are:

$$\nu_{21} = - s_{12}' / s_{11}'$$

$$\nu_{31} = - s_{13}' / s_{11}'$$

These results reduce to those of Case 1) when $\psi = 0$, and to those of Case 2) when $\chi = 0$.

Bulk Modulus

The bulk modulus, or compressibility, κ, is often associated with considerations requiring use of the Poisson's ratio. It is defined as the hydrostatic pressure required to bring about a unit relative change of volume of a substance; it is always positive. For solids of the most general anisotropy, κ is found from the relation

$$[(s_{11} + s_{22} + s_{33}) + 2\,(s_{23} + s_{13} + s_{12})] = 1 / \kappa.$$

For the hexagonal system this reduces to:

$$[(2\,s_{11} + s_{33}) + 2\,(2\,s_{13} + s_{12})] = 1 / \kappa.$$

Application to Piezoceramics

The poling state of piezoceramics nearly always encountered in present commercial practice is either parallel, or lateral, to the major surfaces of the device. This is because the effective piezoelectric coupling is thereby maximized by the electrode placements. Newer configurations, currently under development for microelectromechanical structures (MEMS) applications, utilize more general orientations that take advantage of the achievable differences in Poisson's ratios in different directions. Table 2 gives some representative examples, based on the relations derived above; entries are computed from data in Refs. 6 and 7.

TABLE 2. POISSON'S RATIO, YOUNG'S MODULUS, AND COMPRESSIBILITY OF SELECTED PIEZOCERAMICS.

COMPOSITION	$\theta°,\psi°$	ν_{21}	ν_{31}	Y	κ
$Ba\ Ti\ O_3$	0,0	0.305	0.333	117.0	106.3
PZT-4	45,0	0.380	0.380	81.3	92.9
PZT-5A	0,45	0.380	0.392	58.6	89.1
PZT 52/48	45,45	0.401	0.354	63.7	93.5
PZT 65/35	0,0	0.290	0.395	110.3	95.6
$Pb_{0.76}\ Ca_{0.24}\ Ti\ O_3$	45,0	0.399	0.399	136.1	69.6
$Pb_{0.96}\ La_{0.04}\ Ti\ O_3$	0,45	0.232	0.163	147.2	81.4
$Pb_{0.89}\ Nd_{0.11}\ Ti\ O_3$	45,45	0.235	0.262	149.4	94.0

[Y and κ in GPa]

Conclusions

Poisson's ratio, with respect to rotated coordinate axes, for hexagonal materials, and particularly, poled ferroelectric ceramics, has been obtained. All results are independent of rotations about the six-fold axis. A number of simple cases are of particular interest:

- For longitudinal extension in the basal plane, $\psi = 0$:

  When $\theta = 0$: $\nu_{21} = - s_{12} / s_{11}$; $\nu_{31} = - s_{13} / s_{11}$

  When $\theta = \pi/4$: $\nu_{21} = \nu_{31} = - (s_{12} + s_{13}) / 2 s_{11}$

- For longitudinal extension at an angle ψ from the basal plane:

  When $\theta = 0$; $\psi = \pi/4$: $\nu_{21} = - 2 (s_{12} + s_{13}) / (s_0 + s_{44})$

  $\nu_{31} = - (s_0 - s_{44}) / (s_0 + s_{44})$; $s_0 = (s_{11} + s_{33} + 2 s_{13})$

  When $\theta = \pi/4$; $\psi = \pi/4$: $s_2 = (s_{11} + s_{33} - (s_{44} + 2 s_{13}))$

  $\nu_{21} = - [4 s_{12} + 12 s_{13} + 2 s_2] / [12 s_{11} + 4 s_{33} - 3 s_2]$

  $\nu_{31} = - [8 s_{12} + 8 s_{13} + s_2] / [12 s_{11} + 4 s_{33} - 3 s_2]$

  When $\psi = \pi/4$; $\chi = \pi/4$: $s_2 = (s_{11} + s_{33} - (s_{44} + 2 s_{13}))$

  $\nu_{21} = \nu_{31} = - [s_{12} + 3 s_{13} + s_2 / 2] / [2 (s_{11} + s_{33}) - s_2]$

- For longitudinal extension along the six-fold axis:

  $\nu_{21} = \nu_{31} = - s_{13} / s_{33}$

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2800 Powder Mill Road
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Dir, CECOM Night Vision/
Electronic Sensors Directorate
ATTN: AMSEL-RD-NV-D
(1) Fort Belvoir, VA 22060-5677

Dir, CECOM Intelligence and
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(1) Warrenton, VA 22186-5100

Cdr, Marine Corps Liaison Office
ATTN: AMSEL-LN-MC
(1) Fort Monmouth, NJ 07703-5033